

4-(1-ethoxy ethyl)-Guaiacol

Inchi:	InChI=1S/C11H16O3/c1-4-14-8(2)9-5-6-10(12)11(7-9)13-3/h5-8,12H,4H2,1-3H3
InchiKey:	WVKDLJJPYDSJLFF-UHFFFAOYSA-N
Formula:	C11H16O3
SMILES:	CCOC(C)c1ccc(O)c(OC)c1
Mol. weight [g/mol]:	196.24

Physical Properties

Property code	Value	Unit	Source
gf	-222.54	kJ/mol	Joback Method
hf	-492.34	kJ/mol	Joback Method
hfus	22.53	kJ/mol	Joback Method
hvap	60.46	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.498		Crippen Method
mcvol	159.700	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
ripol	2213.00		NIST Webbook
ripol	2213.00		NIST Webbook
tb	607.76	K	Joback Method
tc	822.95	K	Joback Method
tf	393.85	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.04	J/molxK	607.76	Joback Method
cpg	421.09	J/molxK	643.62	Joback Method
cpg	434.37	J/molxK	679.49	Joback Method
cpg	446.91	J/molxK	715.35	Joback Method
cpg	458.77	J/molxK	751.22	Joback Method
cpg	469.97	J/molxK	787.08	Joback Method
cpg	480.56	J/molxK	822.95	Joback Method
dvisc	0.0008428	Paxs	393.85	Joback Method

dvisc	0.0003534	Paxs	429.50	Joback Method
dvisc	0.0001693	Paxs	465.15	Joback Method
dvisc	0.0000901	Paxs	500.81	Joback Method
dvisc	0.0000521	Paxs	536.46	Joback Method
dvisc	0.0000323	Paxs	572.11	Joback Method
dvisc	0.0000212	Paxs	607.76	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R338608&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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